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COMMENTS ON ANOVA CALCULATIONS FOR MESSY DATA†

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Abstract

Description is given of the relationship of certain forms of the  $R( )$  notation for reductions in sums of squares and the sums of squares in the weighted means analysis. A small numerical example illustrates the relationship.

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# COMMENTS ON ANOVA CALCULATIONS FOR MESSY DATA<sup>†</sup>

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## Introduction

Data can be described as "messy" when each sub-most cell of the classifications does not have the same number of observations. This includes the possibility that some, maybe many, of the cells may have no data at all. Thus "messy" data are what are more usually called unbalanced, non-orthogonal, or unequal-subclass-numbers data, including the possibility of empty cells.

Models for the analysis of variance (ANOVA) of messy data are usually represented by the familiar equation

$$\underline{y} = \underline{X}\underline{b} + \underline{e} , \quad (1)$$

where  $\underline{y}$  is the vector of data,  $\underline{X}$  is a matrix of known values,  $\underline{b}$  is a vector of unknown parameters to be estimated and  $\underline{e}$  is a vector of error terms. The reduction in sum of squares due to fitting such a model (either by least squares or, under normality assumptions, by maximum likelihood) is

$$R(\underline{b}) = \underline{y}'\underline{X}(\underline{X}'\underline{X})^{-1}\underline{X}'\underline{y} \quad (2)$$

where

$$\underline{X}'\underline{X}(\underline{X}'\underline{X})^{-1}\underline{X}'\underline{X} = \underline{X}'\underline{X} \quad (3)$$

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The normal equations are

$$\tilde{X}'\tilde{X}\tilde{b}^0 = \tilde{X}'\tilde{y} \quad (4)$$

with solution

$$\tilde{b}^0 = (\tilde{X}'\tilde{X})^{-1}\tilde{X}'\tilde{y} . \quad (5)$$

Although (5) is pro forma a solution to (4), the computational procedure for deriving (5) that is usually adopted is to amend the non-full rank equations (4) in some manner that yields a full rank representation of them. Then from the solution of this full rank representation a solution  $\tilde{b}^0$  can be easily obtained. Two commonly used methods of amending the full rank equations are those of making certain elements of the solution vector  $\tilde{b}^0$  add to zero; or of putting certain elements equal to zero (see, for example, Searle [1971, Sec. 5.7]).

Having obtained  $\tilde{b}^0$ , it can then be utilized in (2) to give

$$\begin{aligned} R(\tilde{b}) &= \tilde{b}^0' \tilde{X}' \tilde{y} \\ &= \text{inner product of solution vector and right-hand sides of normal equations} \\ &= \text{i.p.o. solutions and r.h.s.'s} . \end{aligned} \quad (6)$$

A simple extension of  $R(\tilde{b})$  is to define  $R(\tilde{b}_1 | \tilde{b}_2)$  as the difference between  $R(\tilde{b}_1, \tilde{b}_2)$  for fitting  $\tilde{y} = \tilde{X}_1 \tilde{b}_1 + \tilde{X}_2 \tilde{b}_2 + \tilde{e}$  and  $R(\tilde{b}_2)$  for fitting  $\tilde{y} = \tilde{X}_2 \tilde{b}_2 + \tilde{e}$ . Then from (2)

$$R(\tilde{b}_1 | \tilde{b}_2) = R(\tilde{b}_1, \tilde{b}_2) - R(\tilde{b}_2) \quad (7)$$

$$= \tilde{y}' \begin{bmatrix} \tilde{X}_1 & \tilde{X}_2 \end{bmatrix} \begin{bmatrix} \tilde{X}_1' \tilde{X}_1 & \tilde{X}_1' \tilde{X}_2 \\ \tilde{X}_2' \tilde{X}_1 & \tilde{X}_2' \tilde{X}_2 \end{bmatrix}^{-1} \begin{bmatrix} \tilde{X}_1' \\ \tilde{X}_2' \end{bmatrix} \tilde{y} - \tilde{y}' \tilde{X}_2 (\tilde{X}_2' \tilde{X}_2)^{-1} \tilde{X}_2' \tilde{y} . \quad (8)$$

The 2-Way Classification

The familiar 2-way cross-classification (rows-by-columns) is a convenient framework for illustrating some features of calculating sums of squares denoted by  $R(\underline{b})$ . The model equation for  $a$  rows and  $b$  columns and  $n_{ij}$  observations in the  $i^{th}$  row and  $j^{th}$  column can be taken as

$$y_{ijk} = \mu + \alpha_i + \beta_j + \gamma_{ij} + e_{ijk} \quad (9)$$

for  $i = 1, \dots, a$ ,  $j = 1, \dots, b$  and  $k = 1, \dots, n_{ij}$  with  $n_{ij} \geq 0$ . In matrix notation, commensurate with using (7), we write (9) as

$$\underline{y} = \mu \underline{1} + \underline{X}_\alpha \underline{\alpha} + \underline{X}_\beta \underline{\beta} + \underline{X}_\gamma \underline{\gamma} + \underline{e} \quad (10)$$

where  $\underline{1}$  is a vector of ones, the  $\underline{X}$ 's are incidence matrices and  $\underline{\alpha}$ ,  $\underline{\beta}$  and  $\underline{\gamma}$  are vectors of the  $\alpha_i$ 's,  $\beta_j$ 's and  $\gamma_{ij}$ 's respectively. In this situation the two analysis of variance tables that can be calculated for data consisting of  $N$  observations in  $s$  different cells are as outlined in Table 1.

TABLE 1: The usual 2 analyses of variance

<u>Analysis 1</u>		<u>Analysis 2</u>	
<u>Sum of Squares</u>	<u>d.f.</u>	<u>Sum of Squares</u>	<u>d.f.</u>
$R(\mu)$	1	$R(\mu)$	1
$R(\underline{\alpha} \mu)$	$a-1$	$R(\underline{\beta} \mu)$	$b-1$
$R(\underline{\beta} \mu, \underline{\alpha})$	$b-1$	$R(\underline{\alpha} \mu, \underline{\beta})$	$a-1$
$R(\underline{\gamma} \mu, \underline{\alpha}, \underline{\beta})$	$s-(a+b-1)$	$R(\underline{\gamma} \mu, \underline{\alpha}, \underline{\beta})$	$s-(a+b-1)$
<u>SSE</u>	<u><math>N-s</math></u>	<u>SSE</u>	<u><math>N-s</math></u>
<u><math>SST = \underline{y}'\underline{y}</math></u>	<u><math>N</math></u>	<u><math>SST = \underline{y}'\underline{y}</math></u>	<u><math>N</math></u>

Details are available in Searle [1971, Chapter 7].

One term not occurring in Table 1 is

$$R(\underline{\alpha}|\mu, \underline{\beta}, \underline{\gamma}) = R(\mu, \underline{\alpha}, \underline{\beta}, \underline{\gamma}) - R(\mu, \underline{\beta}, \underline{\gamma}) . \quad (11)$$

Although this formal definition is in keeping with (7), the expression on the right-hand side of (11) is identically equal to zero. This is because  $R(\mu, \alpha, \beta, \gamma)$  is the reduction in sum of squares due to fitting the model (10), which is well-known to be

$$R(\mu, \alpha, \beta, \gamma) = \sum_{i=1}^a \sum_{j=1}^b n_{ij} \bar{y}_{ij}^2 \quad (12)$$

where  $\bar{y}_{ij} = \frac{\sum_{k=1}^{n_{ij}} y_{ijk}}{n_{ij}}$ . And  $R(\mu, \beta, \gamma)$  in (11) is the reduction in sum of squares due to fitting  $y_{ijk} = \mu + \beta_j + \gamma_{ij} + e_{ijk}$ . This model is indistinguishable from the 2-way nested (hierarchical) model, for which the reduction in sum of squares is well-known (e.g., Searle [1971], p. 252) to be  $\sum_{j=1}^b \sum_{i=1}^{a_j} n_{ij} \bar{y}_{ij}^2$  when  $i = 1, 2, \dots, a_j$ . In our case here,  $a_j = a$  for all  $j$ , and so we have

$$R(\mu, \beta, \gamma) = \sum_{i=1}^a \sum_{j=1}^b n_{ij} \bar{y}_{ij}^2 \quad (13)$$

the same as (12). Substituting (12) and (13) in (11) gives

$$R(\alpha | \mu, \beta, \gamma) \equiv 0. \quad (14)$$

#### Methods of Calculation

Despite the result (14), there are ways of computing what might be called  $R(\alpha | \mu, \beta, \gamma)$  and getting a non-zero value for it. To distinguish this we call it  $R^*(\alpha | \mu, \beta, \gamma)$ , and describe its calculation by first considering the procedure for calculating  $R(\mu, \alpha, \beta, \gamma)$  based on (6).

Correct procedure for calculating  $R(\mu, \alpha, \beta, \gamma)$

- [1] Write out a model with  $\mu$ ,  $\alpha$ ,  $\beta$  and  $\gamma$ .
- [2] Write out normal equations for the model in [1].
- [3] Amend the equations in [2] to be of full rank.
- [4] Solve the equations in [3].
- [5] Calculate  $R(\mu, \alpha, \beta, \gamma) = \text{i.p.o. solutions and r.h.s. of [2], as in (6).}$

The important thing to notice is that calculation of  $R(\mu, \alpha, \beta, \gamma)$  starts from the model [1] containing just  $\mu$ ,  $\alpha$ ,  $\beta$  and  $\gamma$ . This is the principle inherent in (1) and (2) that  $R(b)$  must be calculated from a model that consists of just  $b$ . It seems an obvious principle, but it is violation of this principle that leads to  $R^*(\alpha|\mu, \beta, \gamma)$ . The principle is also evident in the procedure for calculating  $R(\mu, \beta, \gamma)$ .

Correct procedure for calculating  $R(\mu, \beta, \gamma)$

- [11] Write out a model with  $\mu$ ,  $\alpha$ ,  $\beta$ , and  $\gamma$ .
- [11a] Reduce the model in [11] by deleting  $\alpha$ .
- [12] Write out normal equations for the model in [11a].
- [13] Amend the equations in [12] to be of full rank.
- [14] Solve the equations in [13].
- [15] Calculate  $R(\mu, \beta, \gamma) = \text{i.p.o. solutions and r.h.s. of [12], as in (6)}$ .

A consequence of this procedure is that

$$R(\mu, \beta, \gamma) = R(\mu, \alpha, \beta, \gamma) \quad (15)$$

as it should, in accordance with (12) and (13).

The principle that  $R(b)$  be calculated from a model containing just  $b$  is evident here in steps [11] and [11a], comparable to step [1] of calculating  $R(\mu, \alpha, \beta, \gamma)$ . Between them, steps [11] and [11a] lead to a model containing just  $\mu$ ,  $\beta$  and  $\gamma$  and then steps [12] - [15] are exact counterparts of [2] - [5], and so the result is  $R(\mu, \beta, \gamma)$ . In contrast, a computing procedure that has sometimes been adopted can be described as follows.

An incorrect procedure for calculating  $R(\mu, \beta, \gamma)$  that yields  $R^*(\mu, \beta, \gamma)$

- [21] Write out a model with  $\mu$ ,  $\alpha$ ,  $\beta$  and  $\gamma$ .
- [22] Write out normal equations for the model in [21].
- [23] Amend the equations in [22] to be of full rank.
- [23a] Reduce the equations in [23] by deleting  $\alpha$ .
- [24] Solve the equations in [23a].
- [25] Calculate  $R^*(\mu, \beta, \gamma) = \text{i.p.o. solutions and r.h.s. of [23a], similar to (6)}$ .

The result will be that

$$R^*(\mu, \beta, \gamma) \neq R(\mu, \alpha, \beta, \gamma) , \quad (16)$$

in contrast to (15), and hence

$$R^*(\alpha | \mu, \beta, \gamma) = R(\mu, \alpha, \beta, \gamma) - R^*(\mu, \beta, \gamma) \neq 0 \quad (17)$$

in contrast to (14).

The difference between this procedure and the preceding one is that the principle of calculating  $R(\underline{b})$  from a model containing just  $\underline{b}$  is violated. The model here is specified in [21] and contains  $\mu$ ,  $\alpha$ ,  $\beta$  and  $\gamma$ . The normal equations [22] are for that model, they are amended in [23] and then, in [23a], the reduction that arises from deleting  $\alpha$  occurs. But this is a reduction of equations, not of a model as it should be, in order to start from the model consisting of  $\mu$ ,  $\beta$  and  $\gamma$ . In contrast, the reduction in [11a] is of a model, and so is correct and the calculation yields  $R(\mu, \beta, \gamma)$ . But in [23a] the reduction is of some normal equations that have already been amended – and the result is by no means necessarily the same as the correct procedure in [13]. There the model consisting of  $\mu$ ,  $\beta$  and  $\gamma$  is obtained first, as it should be, by reducing the model consisting of  $\mu$ ,  $\alpha$ ,  $\beta$  and  $\gamma$ . In [23a] the reduction occurs at the wrong place, as a reduction of equations. It should always be reduction of a model so as to start the calculating of  $R(\underline{b})$  from the correct model.

Although this discussion is in terms of the 2-way classification it applies quite generally to all linear models. The salient feature is that  $R(\underline{b})$  applies to a model  $\underline{y} = \underline{X}\underline{b} + \underline{e}$  and it must be calculated from (6), as described in the first of the three preceding procedures.

Yates' Weighted Squares of Means

There is one interesting case where calculation of  $R^*(\mu, \beta, \gamma)$ , although not yielding  $R(\mu, \beta, \gamma)$ , does produce something of interest. This is in the 2-way cross-classification, with unequal numbers of observations in the cells, and with all cells fitted; i.e., each cell having at least one observation. Suppose in this situation we amend the normal equations (step [23]) by requiring the solutions to satisfy

$$\sum_{i=1}^a \alpha_i = 0, \quad \sum_{j=1}^b \beta_j = 0, \quad \sum_{i=1}^a \gamma_{ij} = 0 \text{ for all } j, \text{ and } \sum_{j=1}^b \gamma_{ij} = 0 \text{ for all } i. \quad (18)$$

This is the method of amending equations customarily used in balanced data (equal numbers of observations in the subclasses) and it has been carried over into a number of computer routines for unbalanced data. Provided all cells have some data we then have the interesting consequence that for  $SSA_w$  defined as

$SSA_w \equiv$  sum of squares for  $\alpha$ -effects in the weighted squares of means analysis

$$= \sum_{i=1}^a \frac{\left[ \sum_{j=1}^b \bar{y}_{ij\cdot} \right]^2}{\sum_{j=1}^b 1/n_{ij}} - \frac{\left[ \sum_{i=1}^a \frac{\sum_{j=1}^b \bar{y}_{ij\cdot}}{\sum_{j=1}^b 1/n_{ij}} \right]^2}{\sum_{i=1}^a \frac{1}{\sum_{j=1}^b 1/n_{ij}}}, \quad (19)$$

then  $R^*(\alpha|\mu, \beta, \gamma)$  of (17) is

$$R^*(\alpha|\mu, \beta, \gamma) = SSA_w. \quad (20)$$

A full description of the weighted squares of means analysis may be found, for example, in Searle [1971], pp. 369-372.

Yates [1934] described the analysis of which (19) is a part; and many people are aware that (20) provides a convenient way to calculate (19). Despite this,



a formal proof of (20) remains, so far as I know, to be developed. The validity of (20) is often attributed to Yates [1934], as indeed development of (19) is and should be, but careful scrutiny of Yates [1934] does not appear to reveal a formal proof of (20). Yet its validity has been demonstrated in countless examples, one of which follows.

The extension of (20) to k-way classifications for  $k > 2$  seems obvious. Formal proof of such extensions is also required.

### Example

Consider the following data for 2 rows and 3 columns.

TABLE 2: Data

8,13,9	12	7,11	60
11,14,17	14,16	10,11,14,13	120
72	42	66	180

The analyses of variance of Table 2 are shown in Table 3.

TABLE 3: Analyses of variance of data in Table 2

Analysis 1			Analysis 2		
<u>Source</u>	<u>d.f.</u>	<u>s.s.</u>	<u>Source</u>	<u>d.f.</u>	<u>s.s.</u>
$R(\mu)$	1	2160	$R(\mu)$	1	2160
$R(\alpha \mu)$	1	40	$R(\beta \mu)$	2	18
$R(\beta \mu, \alpha)$	2	$19\frac{1}{7}$	$R(\alpha \mu, \beta)$	1	$41\frac{1}{7}$
$R(\gamma \mu, \alpha, \beta)$	2	$\frac{6}{7}$	$R(\gamma \mu, \alpha, \beta)$	2	$\frac{6}{7}$
SSE	9	52	SSE	9	52
SST	15	2272	SST	15	2272

To demonstrate calculation of  $R^*(\alpha|\mu, \beta, \gamma)$  we carry out the steps [21] through [25]. Clearly, [21] is equation (9). Then [22] is

$$\begin{bmatrix}
 15 & 6 & 9 & 6 & 3 & 6 & 3 & 1 & 2 & 3 & 2 & 4 \\
 \hline
 6 & 6 & \cdot & 3 & 1 & 2 & 3 & 1 & 2 & \cdot & \cdot & \cdot \\
 9 & \cdot & 9 & 3 & 2 & 4 & \cdot & \cdot & \cdot & 3 & 2 & 4 \\
 \hline
 6 & 3 & 3 & 6 & \cdot & \cdot & 3 & \cdot & \cdot & 3 & \cdot & \cdot \\
 3 & 1 & 2 & \cdot & 3 & \cdot & \cdot & 1 & \cdot & \cdot & 2 & \cdot \\
 6 & 2 & 4 & \cdot & \cdot & 6 & \cdot & \cdot & 2 & \cdot & \cdot & 4 \\
 \hline
 3 & 3 & \cdot & 3 & \cdot & \cdot & 3 & \cdot & \cdot & \cdot & \cdot & \cdot \\
 1 & 1 & \cdot & \cdot & 1 & \cdot & \cdot & 2 & \cdot & \cdot & \cdot & \cdot \\
 2 & 2 & \cdot & \cdot & \cdot & 2 & \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\
 3 & \cdot & 3 & 3 & \cdot & \cdot & \cdot & \cdot & \cdot & 3 & \cdot & \cdot \\
 2 & \cdot & 2 & \cdot & 2 & \cdot & \cdot & \cdot & \cdot & \cdot & 2 & \cdot \\
 4 & \cdot & 4 & \cdot & \cdot & 4 & \cdot & \cdot & \cdot & \cdot & \cdot & 4
 \end{bmatrix}
 \begin{bmatrix}
 \mu \\
 \alpha_1 \\
 \alpha_2 \\
 \beta_1 \\
 \beta_2 \\
 \beta_3 \\
 \gamma_{11} \\
 \gamma_{12} \\
 \gamma_{13} \\
 \gamma_{21} \\
 \gamma_{22} \\
 \gamma_{23}
 \end{bmatrix}
 =
 \begin{bmatrix}
 180 \\
 60 \\
 120 \\
 72 \\
 42 \\
 66 \\
 30 \\
 12 \\
 18 \\
 42 \\
 30 \\
 48
 \end{bmatrix}
 \quad (21)$$

The next step, [23], is to amend these equations to be of full rank, and doing so by use of (18) gives

$$\begin{bmatrix}
 15 & -3 & 0 & -3 & 2 & 1 \\
 -3 & 15 & 2 & 1 & 0 & -3 \\
 0 & 2 & 12 & 6 & -2 & -2 \\
 -3 & 1 & 6 & 9 & -2 & -3 \\
 2 & 0 & -2 & -2 & 12 & 6 \\
 1 & -3 & -2 & -3 & 6 & 9
 \end{bmatrix}
 \begin{bmatrix}
 \mu \\
 \alpha_1 \\
 \beta_1 \\
 \beta_2 \\
 \gamma_{11} \\
 \gamma_{12}
 \end{bmatrix}
 =
 \begin{bmatrix}
 180 \\
 -60 \\
 6 \\
 -24 \\
 18 \\
 12
 \end{bmatrix}
 \quad (22)$$

Then [23a] reduces the equations by deletion of  $\alpha$ , so leading to

$$\begin{bmatrix} 15 & 0 & -3 & 2 & 1 \\ 0 & 12 & 6 & -2 & -2 \\ -3 & 6 & 9 & -2 & -3 \\ 2 & -2 & -2 & 12 & 6 \\ 1 & -2 & -3 & 6 & 9 \end{bmatrix} \begin{bmatrix} \mu \\ \beta_1 \\ \beta_2 \\ \gamma_{11} \\ \gamma_{12} \end{bmatrix} = \begin{bmatrix} 180 \\ 6 \\ -24 \\ 18 \\ 12 \end{bmatrix} . \quad (23)$$

Solving these equations, as in [24] gives the solution

$$[\mu \quad \beta_1 \quad \beta_2 \quad \gamma_{11} \quad \gamma_{12}] = [12\frac{3}{7} \quad \frac{-3}{7} \quad 1\frac{13}{14} \quad \frac{-6}{7} \quad 1\frac{1}{14}] \quad (24)$$

and then step [25] takes the inner product of this solution vector with the vector on the right-hand side of (23):

$$R^*(\mu, \beta, \gamma) = 12\frac{3}{7}(180) - \frac{3}{7}(6) + 1\frac{13}{14}(-24) - \frac{6}{7}(18) + 1\frac{1}{14}(12) = 2185\frac{5}{7} . \quad (25)$$

To obtain  $R^*(\alpha | \mu, \beta, \gamma)$  of (17) we need  $R(\mu, \alpha, \beta, \gamma)$ . From using the data of Table 2 in (12) this is found to be

$$R(\mu, \alpha, \beta, \gamma) = 2220 . \quad (26)$$

In passing, observe from (13) that  $R(\mu, \beta, \gamma) = 2220$  also, and that this is not the value of  $R^*(\mu, \beta, \gamma)$  in (25). The difference is, in accord with (17),

$$R^*(\alpha | \mu, \beta, \gamma) = 2220 - 2185\frac{5}{7} = 34\frac{2}{7} . \quad (27)$$

And on using (19) we find that

$$SSA_w = \frac{(10 + 12 + 9)^2}{\frac{1}{3} + \frac{1}{1} + \frac{1}{2}} + \frac{(14 + 15 + 12)^2}{\frac{1}{3} + \frac{1}{2} + \frac{1}{4}} - \frac{\left[ \frac{10 + 12 + 9}{\frac{1}{3} + \frac{1}{1} + \frac{1}{2}} + \frac{14 + 15 + 12}{\frac{1}{3} + \frac{1}{2} + \frac{1}{4}} \right]^2}{\left[ \frac{1}{\frac{1}{3} + \frac{1}{1} + \frac{1}{2}} + \frac{1}{\frac{1}{3} + \frac{1}{2} + \frac{1}{4}} \right]} = 34\frac{2}{7} \quad (28)$$

has the same value; i.e.,  $R^*(\alpha | \mu, \beta, \gamma) = SSA_w$ , as in (20).

Notation. In equations (21), (22) and (23), and the solution (24) we have used the symbols  $\mu$ ,  $\alpha$ ,  $\beta$  and  $\gamma$  without distinguishing them from the parameter values shown in the model equation (9). However, the distinction must be recognized, for in truth they do not represent the same thing in all of these equations. These symbols represent solutions to normal equations and adaptations thereof in (21), (22), (23) and (24), whereas in (9) they represent unknown parameter values. Furthermore, those symbols represent different things as between equations (21), (22) and (23). For example, (22) has a unique solution, which on utilizing (18) then also satisfies (21); but there are also many other solutions of (21). And (24), whilst it is the unique solution of (23), is not part of the solution of (21); nor of (22). Modifying the symbols in (22), (23) and (24), perhaps by the addition of superscripts to distinguish the three cases, would emphasize the implied distinctions, but for the sake of notational simplicity has not been done. Nevertheless, the distinctions must not be overlooked.

#### Empty Cells

It is to be emphasized that (20) applies only for the case of all cells filled. When some cells are empty, use and interpretation of equations (18) is very difficult, if not impossible, because for empty cells there are no data on the corresponding  $\gamma$ 's and yet they occur in equations (18). Moreover, of course, the weighted means analysis that yields  $SSA_w$  does not exist for data having empty cells and so any attempt at calculating  $R^*(\alpha|\mu, \beta, \gamma)$  utilizing (18) cannot yield  $SSA_w$ .

#### References

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